Note for Nikiforov's two conjectures on the energy of trees*

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Abstract

The energy E of a graph is defined to be the sum of the absolute values of its eigenvalues. Nikiforov in "V. Nikiforov, The energy of C_4 -free graphs of bounded degree, Lin. Algebra Appl. 428(2008), 2569–2573" proposed two conjectures concerning the energy of trees with maximum degree $\Delta \leq 3$. In this short note, we show that both conjectures are true.

Key words: energy of a graph, conjecture, tree

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Let G be a graph on n vertices and $\lambda_1, \lambda_2, \dots, \lambda_n$ be the eigenvalues of its adjacency matrix. The value $E(G) = |\lambda_1| + \dots + |\lambda_n|$ is defined as the energy of G, which has been studied intensively, see [1, 3] for a survey.

In [5], Nikiforov proposed two conjectures on the energy of trees. In order to state and prove them, we need the following notations and terminology.

The complete d-ary tree of height h-1 is denoted by C_h , which is built up inductively as follows: C_1 is a single vertex and C_h has d branches C_{h-1}, \dots, C_{h-1} . See Figure 1 for examples. It is convenient to set C_0 as the empty graph.

Let $\mathcal{T}_{n,d}$ be the set of all trees with n vertices and maximum degree d+1. We define a special tree $T_{n,d}^*$ as follows (see also [4]):

Definition 1 $T_{n,d}^*$ is the tree with n vertices that can be decomposed as in Figure 2

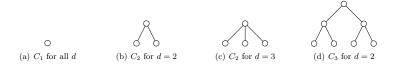


Figure 1 Some small complete d-ary trees.

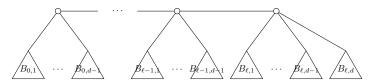


Figure 2 Tree $T_{n,d}^*$.

with $B_{k,1}, \dots, B_{k,d-1} \in \{C_k, C_{k+2}\}$ for $0 \le k < l$ and either $B_{l,1} = \dots = B_{l,d} = C_{l-1}$ or $B_{l,1} = \dots = B_{l,d} = C_l$ or $B_{l,1}, \dots, B_{l,d} \in \{C_l, C_{l+1}, C_{l+2}\}$, where at least two of $B_{l,1}, \dots, B_{l,d}$ equal C_{l+1} . This representation is unique, and one has the "digital expansion"

$$(d-1)n + 1 = \sum_{k=0}^{l} a_k d^k, \tag{1}$$

where $a_k = (d-1)(1+(d+1)r_k)$ and $0 \le r_k \le d-1$ is the number of $B_{k,i}$ that are isomorphic to C_{k+2} for k < l, and

- $\bullet a_l = 1 \quad if \quad B_{l,1} = \cdots = B_{l,d} = C_{l-1},$
- $a_l = d$ if $B_{l,1} = \cdots = B_{l,d} = C_l$,
- or otherwise $a_l = d + (d-1)q_l + (d^2-1)r_l$, where $q_l \ge 2$ is the number of $B_{l,i}$ that are isomorphic to C_{l+1} and r_l is the number of $B_{l,i}$ that are isomorphic to C_{l+2} .

Let \mathcal{B}_n denote the tree constructed by taking three disjoint copies of the complete 2-ary tree of height h-1, i.e., C_n , and joining an additional vertex to their roots (i.e., vertices of height zero). In the end of [5], Nikiforov formulated two conjectures as follows:

Conjecture 2 The limit

$$c = \lim_{n \to \infty} \frac{E(\mathcal{B}_n)}{3 \cdot 2^{n+1} - 2}$$

exists and c > 1.

Conjecture 3 Let $\epsilon > 0$. If T is a sufficiently large tree with $\Delta(T) \leq 3$, then $E(T) \geq (c - \epsilon)|T|$.

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Nikiforov mentioned that empirical data given in [2] seem to corroborate these conjectures, but apparently new techniques are necessary to prove or disprove them. We will give confirmative proofs for both Conjecture 2 and Conjecture 3.

We first state two known lemmas from [4], which will be needed in the sequel.

Lemma 4 [4]. Let n and d be positive integers. Then $T_{n,d}^*$ is the unique (up to isomorphism) tree in $\mathcal{T}_{n,d}$ that minimizes the energy.

Lemma 5 [4]. The energy of $T_{n,d}^*$ is asymptotically

$$E(T_{n,d}^*) = \alpha_d \cdot n + O(\ln n),$$

where

$$\alpha_d = 2\sqrt{d}(d-1)^2 \left(\sum_{\substack{j \ge 1 \\ j \equiv 0 \pmod{2}}} d^{-j} \left(\cot \frac{\pi}{2j} - 1 \right) + \sum_{\substack{j \ge 1 \\ j \equiv 1 \pmod{2}}} d^{-j} \left(\csc \frac{\pi}{2j} - 1 \right) \right)$$
 (2)

is a constant that only depends on d.

d	$lpha_d$
2	1.102947505597
3	0.970541979946
4	0.874794345784
5	0.802215758706
6	0.744941364903
7	0.698315075830
8	0.659425329682
9	0.626356806404
10	0.597794680849
20	0.434553264777
50	0.279574397741
100	0.198836515295

Table 1 Some numerical values for the constant α_d .

With the above two lemmas, the two conjectures can be proved very easily as follows.

Theorem 6 The limit

$$c = \lim_{n \to \infty} \frac{E(\mathcal{B}_n)}{3 \cdot 2^{n+1} - 2}$$

exists and c > 1.

Proof. We just need to notice that \mathcal{B}_n is exactly the tree $T^*_{3\cdot 2^{n+1}-2,2}$ with $l=n,\ B_{k,1}=C_k$ for $0 \leq k < l,\ B_{l,1}=B_{l,2}=C_n$. Therefore, by Lemma 5 and Table 1 we have

$$\lim_{n \to \infty} \left(\frac{E(\mathcal{B}_n)}{3 \cdot 2^{n+1} - 2} \right) = \lim_{n \to \infty} \left(\alpha_2 + \frac{O(\ln(3 \cdot 2^{n+1} - 2))}{3 \cdot 2^{n+1} - 2} \right) = \alpha_2 > 1.$$

In fact, from Lemmas 4 and 5 we have that for any $T \in \mathcal{T}_{n,d}$,

$$E(T) \ge E(T_{n,d}^*) = \alpha_d \cdot n + O(\ln n).$$

Therefore, we obtain

Theorem 7 Let $\epsilon > 0$. If T is a sufficiently large tree with $\Delta(T) = d + 1$, then $E(T) \geq (\alpha_d - \epsilon)|T|$, where α_d is given in Equ.(2).

Letting d=2, we get

Corollary 8 Let $\epsilon > 0$. If T is a sufficiently large tree with $\Delta(T) = 3$, then $E(T) \ge (\alpha_2 - \epsilon)|T|$, where α_2 is given in Equ.(2).

Recall that a hypoenergetic graph of order n is such that E(G) < n, whereas it is strongly hypoenergetic if E(G) < n - 1. We have the following easy remarks:

Remark 1: From Lemma 5 and Table 1, one can see that there is neither strongly hypoenergetic tree nor hypoenergetic tree of order n and maximum degree Δ for $\Delta \leq 3$ and any suitable large n.

Remark 2: From Lemma 5 and Table 1, one can also see that there are both hypoenergetic trees and strongly hypoenergetic trees of order n and maximum degree Δ for $\Delta \geq 4$ and any suitable large n.

References

- [1] I. Gutman, Topology and stability of conjugated hydrocarbons: The dependence of total π -electron energy on molecular topology, *J. Serb. Chem. Soc.* 70 (2005), 441–456.
- [2] I. Gutman, On graphs whose energy exceeds the number of vertices, *Lin. Algebra Appl.* 429(11-12) (2008), 2670–2677.
- [3] I. Gutman, X. Li, J. Zhang, Graph Energy, in: M. Dehmer, F. Emmert-Streib (Eds.), Analysis of Complex Networks: From Biology to Linguistics, Wiley-VCH Verlag, Weinheim, 2009, pp.145-174.

- [4] C. Heuberger, S. Wagner, Chemical tress minimizing energy and Hosoya index, J. $Math.\ Chem.\ 46(1)\ (2009),\ 214–230.$
- [5] V. Nikiforov, The energy of C_4 -free graphs of bounded degree, $Lin.\ Algebra\ Appl.\ 428\ (2008),\ 2569–2573.$